Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 41.7 days

Global applicability domain: Inside

Local applicability domain index: 5.34e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

Image not found
Phenanthrene, trimethyl-
Measured: 26200
Predicted: 75.6

Image not found
1-Methyl phenanthrene
Measured: 1370
Predicted: 36.9

Image not found
2-Methylphenanthrene
Measured: 1370
Predicted: 25.0

Image not found
9-Methylanthracene
Measured: 364000
Predicted: 144

Image not found
Tetralin
Measured: 120
Predicted: 12.2